



Workshops and Conferences

Workshops and Conferences

As a part of its outreach, the ISCR hosts and sponsors various workshops and conferences throughout the year. In many cases, the ISCR co-hosts or co-sponsors the event with other organizations internal and external to LLNL. Subject matter may be drawn from any of the wide range of research interests identified by the ISCR.

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Copper Mountain Conference on Iterative Methods, Mar. 30–Apr. 4, 2003, Copper Mountian, CO	NA
Seventh U.S. National Congress on Computational Mechanics, July 27–31, 2003, Albuquerque, NM	NA
AMG Summit, Sept. 29-Oct. 5, 2003, Lake City, CO	NA
International Conference on Preconditioning Techniques for Large Sparse Matrix Problems in Scientific and Industrial Applications, October 27–29, 2003, Napa, CA	NA



Synopsis of Workshop

Research advances in computational science technology have truly made simulation an equal partner with theory and experiment in understanding physical phenomena. Simulation is increasingly relied upon in government and industry for high impact decisions. As a result, computational scientists are called upon to solve problems with more complex and coupled physics than ever before. Applications such as fluid dynamics, fusion, electronics, groundwater flow, astrophysics, and combustion are producing coupled models where individual effects were previously studied. In addition, parallel computers with large-storage capacities have paved the way for high-resolution simulations on large-scale domains. The growth in complexity and size of models coupled with the advent of more powerful machines has led to a continued and increasing demand for effective algorithms for solving large-scale systems of nonlinear equations.

The Workshop on Solution Methods for Large-Scale Nonlinear Problems, held August 6-8, 2003, in Livermore, California, brought together many of the most active researchers on both the algorithmic and the applications sides of the area. The workshop was hosted by the Center for Applied Scientific Computing and the Institute for Scientific Computing Research at Lawrence Livermore National Laboratory. Major themes included Newton-Krylov methods, preconditioning techniques, operator-split and fully implicit schemes, continuation methods, and Partial Differential Equation (PDE)-constrained optimization. Applications addressed included fluid dynamics, astrophysics, magnetohydrodynamics, porous media flows, radiation diffusion, and other areas. The workshop was a follow-on to similar workshops on large-scale nonlinear problems held at Utah State University (1989, 1995) and in Pleasanton, California (2000). In the spirit of the earlier workshops, liberal break times in the schedule of talks and discussion sessions encouraged informal interactions among participants. Workshop attendees, mainly from the United States, came from academia (17), government laboratories (25), and industry (2). Each of the three workshop days consisted of several talks followed by a moderated discussion of selected issues.

From the presentations, it was clear that the workhorse methods in the field are still Newton-Krylov methods, in which Newton's method is combined with preconditioned Krylov methods for approximately solving the linear Jacobian systems. Efficient schemes for achieving fast convergence, up to the quadratic convergence of Newton's method, have been realized in a number of applications, leaving "robustification" as the main focus of current research. In particular, a number of workshop talks concentrated on globalization and continuation techniques combined with Newton-Krylov methods. The most commonly applied globalization has been *linesearch* (*backtracking*, *damping*), in which each step direction is that of the approximate solution of the Jacobian system and the step length is chosen to give desirable progress toward a solution. *Trust region*

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methods offer an alternative approach, in which each step is taken within a "region of trust" of the local linear model around the current approximate solution. Trust-region implementations of Newton's method combined with the conjugate gradient method (known as truncated Newton methods) have been applied to large-scale optimization problems for some time. In contrast, trust-region globalizations of more general Newton-Krylov methods have not often been used in the past; however, they have recently received attention. Pseudo-transient continuation methods, which have been used in computational fluid dynamics for some years, are now starting to be invoked in other application areas such as groundwater flow. Similarly, parameter continuation methods, which have been used for some time in certain applications, are enjoying broader usage in applications with Newton's method. Systematic comparison of all of these robustification techniques has begun, and further understanding of which method is best for a particular problem is a subject of active research.

Other workshop talks discussed new advances in the use of Newton's method. One such advance is the development of theory for extensions of the method to certain classes of non-smooth nonlinear functions. Using the concept of generalized derivatives, convergence of Newton's method has been shown for these functions, both with and without pseudo-transient continuation. Another advance is in the use of automatic differentiation for efficiently generating accurate Jacobian-vector products within a Newton-Krylov method; this has shown computational speed advantages over finite-difference approximations for fluid dynamics problems. Additionally, initial results were given for applying a two-grid technique that transfers nonlinearities to a coarser resolution version of the original problem. Lastly, there have been new developments in globalized tensor-Krylov methods, which can be regarded as extensions of Newton-Krylov methods that incorporate limited second-order information. Recently developed globalizations, in combination with certain extensions of the Generalized Minimal Residual (GMRES) method, provide robustness and efficiency while allowing the superlinear convergence associated with direct tensor methods on singular and illconditioned problems.

Preconditioning for both nonlinear and linear problems continues to be an important area of research. Further advances in preconditioning the nonlinear problem via a nonlinear additive Schwarz approach were outlined, including three-dimensional and parallel results on computational fluid dynamics problems. Preconditioning the linear Jacobian systems continues to be a primary requirement for the success of Newton-Krylov methods on large-scale problems. An application that had significant interest at the workshop and which has benefited from advances in preconditioning is fusion simulation. Application of Newton-Krylov methods along with the development of effective preconditioning has allowed a move to implicit formulations for some problem classes in this field. These formulations allow for larger time steps that are no longer



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limited to tracking the fastest wave in the system. Extensions of these approaches were also given for the more complicated case of implicit formulations of fusion problems on adaptive meshes. In astrophysics, sparse approximate inverse preconditioners have been developed for multigroup flux-limited diffusion of neutrinos for core-collapse supernovae simulations. These preconditioners have enabled use of Newton-Krylov methods and thus larger time steps for these problems.

Talks from applications scientists reflected the incorporation of these algorithmic advances into scientific simulation codes. In particular, groundwater and geomechanics codes are being coupled together as are shallow water and groundwater simulators. Although these couplings are not all yet fully implicit, nonlinear couplings between the relevant effects can now be studied. In the case of fully implicit formulations of shallow water problems, improved preconditioning and nonlinear solvers allow simulation of hurricanes with much larger time steps than previously could be used. In other applications, preconditioned Newton-Krylov methods have enabled progress in simulation of combustion chemistry and also in modeling phase transitions in smart materials that previously were intractable.

Advances in Newton-Krylov methods have also benefited shape optimization applications, in which the typical PDE solver is now part of a constraint that must be completed for each iteration of the optimization method. Advances in this field have developed by viewing the optimization problem as a large system where the optimization and constraints are handled "all-at-once" with a Newton-Krylov method applied to a system comprised of the objective and the PDE constraints.

Each of the three workshop days ended with a moderated discussion. The discussion on the first day dealt with robustness and failure of nonlinear solvers. The session began with a review of types of failure, including divergence or stagnation of the iterates, convergence to a local norm minimizer that is not a solution, failure of the linear solver to produce adequate linear residual reduction, and convergence to a "wrong" solution, such as a steady state that is dynamically unstable or which violates physical constraints. This was followed by a discussion of causes, symptoms, and possible remedies for various failure modes, together with the general question of how to construct nonlinear solver algorithms to prevent failure if possible and to terminate with useful diagnostic information otherwise. The session concluded with a brief discussion of experiences with several globalization methods (including continuation) and their relative effectiveness in practice.

The second day's discussion was on tolerances, stopping criteria, and related accuracy/efficiency considerations for nonlinear solvers. This discussion initially focused on fully implicit methods for time-dependent problems, first reviewing their merits and

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disadvantages relative to explicit and semi-implicit methods and then addressing the issue of stopping tolerances for the nonlinear residuals associated with the implicit equations that are sufficient to ensure desired accuracy. In general, participants felt that a relative stopping criterion such as 10^{-5} on the nonlinear residual norm worked well in most instances, although some preferred absolute tolerances such as 10^{-5} or 10^{-6} in some applications. The next focus of the discussion was on choosing the difference step in finite-difference approximations of Jacobian-vector products in "matrix-free" Newton-Krylov implementations. Participants commented on their experiences with several previously proposed choices, with some agreement that difference-step formulas should take into account inner products as well as norms of the relevant vectors. In conclusion, the discussion touched on the issue of choosing the relative residual norm tolerances (the *forcing terms*) for approximately solving Jacobian systems in order to enhance efficiency and perhaps robustness as well. Participants reported a variety of experiences, with effective choices in particular applications ranging from adaptive formulations to relatively large (10^{-1}) and small (10^{-4}) constant choices.

The third day's discussion was on algorithms and architectures. The discussion centered on what nonlinear solver software writers and algorithm designers need to pay attention to in order to take advantage of upcoming architectures. The two main consensus items for this question were: careful use of data, so that cache hierarchies can be exploited and data reuse maximized; and fault tolerance in implementations. It was noted that with the large numbers of processors on platforms such as the new ASCI machines and Blue Gene/Light, it will be likely that some number of processors will fail and drop out of a simulation unexpectedly. Implementations of algorithms for these machines will need to tolerate these faults and robustly solve for solutions.

A poster session held on the evening of the second day highlighted the work of students attending the meeting as well as software packages offering robust implementations of Newton-Krylov methods and other nonlinear solvers. The student posters reflected a breadth of work in the field, including solvers for electrical tunneling, optimization methods for groundwater remediation, globalization of Newton-Krylov methods for the Navier-Stokes equations, and variants of Newton-Krylov methods for problems with expensive nonlinear function evaluations. The software posters provided information on the Sandia package NOX, the Lawrence Livermore package SUNDIALS, and the suite of packages offered through the TOPS (Terascale Optimal PDE Simulations) SciDAC project including the Argonne package PETSc. All of these packages are available to the public and offer various functionalities in addition to Newton-Krylov solvers.

Although the presentations at the workshop reflected significant advances in the field of nonlinear solvers, many challenges still remain. Robust solvers for problems discretized with discontinuous Galerkin methods continue to be an open research area, as does



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productive use of multiple-grid levels in nonlinear solvers. Development of nonlinear multigrid and two-grid methods has shown promise, but the robustness and efficiency gains seen on linear problems still have not appeared in the nonlinear realm. Fault tolerant implementation of nonlinear solvers also remains as an important open area.

The field of solution methods for large-scale nonlinear problems is an active research area vital to simulation technology. Advances in nonlinear solver algorithms are helping to push back the frontiers of science in many applications. Interested researchers can see more of this field in sessions on nonlinear solvers at the Copper Mountain Conference on Iterative Methods March 28–April 2, 2003, and at a mini-symposium (submitted) at the Society of Industrial and Applied Mathematics (SIAM) 2004 annual meeting. More information about the workshop described above can be found at www.llnl.gov/casc/workshops/nonlinear_2003 where abstracts and PDF files for many presentations are archived.

Advanced Scientific Computing Requirements Workshop

Synopsis of Workshop

The Advanced Scientific Computing Requirements Workshop was held October 8–9, 2003, at the Crystal City Hilton in Arlington, Virginia. Approximately 95 participants, representing the U.S. Department of Homeland Security (DHS), national laboratories, federal agencies, academia, and industry convened to learn about DHS mission needs and identify mathematics and computer science research and development topic areas to address them.

The Advanced Scientific Computing (ASC) R&D program is part of the Science and Technology (S&T) Directorate within DHS. This program funds R&D to develop enabling computational technologies that will be deployed in the next generation of operational tools designed to simulate and understand physical and biological phenomena for homeland security applications. The ASC program also funds R&D for large-scale data management and integration. These capabilities will be used to improve scenario planning and emergency response, to design better radiation and biological detectors for border protection, to enable vulnerability assessments and consequence analyses for infrastructure protection, and to accelerate information extraction and data assimilation for threat analysis and attribution.

The workshop was organized around six "portfolios" in the S&T Directorate that exist to lead technology development for the operational directorates in DHS. These are the Borders and Transportation Security (BTS) Portfolio, the Emergency Preparedness and Response (EP&R) Portfolio, the Critical Infrastructure Protection (CIP) Portfolio, the Threat Verification, Testing, and Assessment (TVTA) Portfolio, the Chemical and Biological Countermeasures (ChemBio) Portfolio, and the Radiological and Nuclear Countermeasures (Rad/Nuc) Portfolio. Each day of the two-day workshop was structured to provide presentations associated with three of the portfolios in the morning followed by breakout sessions in the afternoon to consider R&D requirements for those portfolios.

Each morning's presentations included overviews for the day's portfolios, talks by DHS operational directorate staff to illustrate mission activities that rely on advanced technology, and presentations by R&D technologists working in applicable technology domains. The afternoon breakouts were organized along portfolio lines but further subdivided to emphasize either modeling and simulation or data sciences. In the breakouts, DHS technology users engaged in roundtable brainstorming with technology developers to identify and refine technology requirements for DHS operational missions.

Going into the workshop planning stage, the ASC program had already identified DHS needs for modeling and simulation and various data-science-related technologies. The workshop served to materially refine and expand these needs and enabled the development of a better sense of the impact that various technologies will have across

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the mission space of DHS. Several data-science technologies—including information sharing and dissemination, data fusion and heterogeneous database integration, and information extraction—were revealed to have across-the-board utility within the portfolios. Likewise, discrete event simulation technology and visualization/visual analytics were needs shared among all of the portfolios. Other technologies had widespread if not universal applicability within the portfolios, including continuum simulations, data-driven simulations, decision support technology, collaborative technology, and geographic information systems. All results from the workshop are being compiled into a final report that will present conclusions as well as more detailed discussions of research opportunities for the ASC program.

Workshop participants, DHS representatives in particular, considered the event a great success, so much so that the workshop is looked on as a model for future requirements development activities. This outcome follows directly from the thorough preparatory efforts in the weeks preceding the workshop by the Program Committee, the Organizing Committee, and the Krell Institute, which was contracted to manage logistics and support planning activities.

As the ten-member Program Committee (senior scientists and technology managers from federal laboratories, academia, and industry) developed the workshop agenda and identified respected speaker and participant pools, the Organizing Committee (LLNL and Krell Institute staff) completed an intensive schedule of trips to Washington DC to interview portfolio managers and their staff. The tangible results of these interviews were the portfolio overviews prepared by the Organizing Committee and presented by portfolio managers at the workshop. Less tangible, but no less important, was the knowledge-base developed of the mission needs and potentially applicable technology domains that permitted the workshop to begin with the primary focus areas already identified. This conferred considerable benefit by maximizing workshop productivity, an important consideration given that the duration of the workshop was necessarily limited to minimize the time commitment from participants.

The Krell Institute, in addition to participating in developing the content of the workshop, handled all logistics for the workshop and also developed the workshop Web site. Krell staff were highly responsive in all tasks and generously lent their expertise wherever they could add value, before, during, and after the workshop.